APPENDIX C

DATA SHEETS FOR CHEMICALS WITH HAZARD-INDEX RANKING: LOW

Chemical Name	Hazard Index: Low
Common Name: allyl isothiocyanate	
Empirical Formula: C4H5NS	CAS Number: 57-06-7

Sorptive Properties

Filter Performance Index:	Effective
Physical Adsorption:	strong adsorption on activated carbon, low water solubility, desorption may decrease or be delayed with increasing relative humidity and adsorbed water.
Chemisorption:	unknown

Physical Properties

Molecular Weight:	99.16
Boiling Point:	150C
Vapor Pressure:	ca. 5 mm Hg at 25 C, antoine: T=283-323 K, A=-0.127508 B=161.415 C=-217.945 (T=K, LogP=bar, NIST)
Volatility:	
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	
Solubility in Water:	<0.1 mg/mL at 19 C
Liquid Density:	1.015 g/cm3

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook
2. www.fisher1.com

Chemical Name	Hazard Index: Low
Common Name: arsenic trichloride Empirical Formula: AsCl3	CAS Number: 7784-34-1

Sorptive Properties

Filter Performance Index: Marginal

Physical Adsorption: Strong to moderate adsorption on activated carbon.

Chemisorption: Possible removal by NBC filters due to hydrolysis and reaction with metal impregnants

Physical Properties

Molecular Weight:	181.28
Boiling Point:	130 C
Vapor Pressure:	ca. 11 mm Hg at 25 C, antoine: T=261.7-403.5 K, A=4.47547 B=1620.019 C=-41.362 (T=K, LogP=bar, NIST))
Volatility:	6.25 (air=1)
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	49.06 cal/g
Solubility in Water:	
Liquid Density:	2.163 g/mL

Toxicity

ACGIH TLV-TWA: 0.2 mg (as)/m3	NIOSH REL-TWA:	OSHA PEL: 0.01 mg/m3
ACGIH TLV-STEL:	NIOSH REL-STEL: 0.002 mg/m3	

References

1. NIST Chemistry WebBook
2. Extremely Hazardous Substances, superfund Chemical Profiles, EPA
Hazardous Chemical Data Book, Weiss, 1986

Chemical Name	Hazard Index: Low
Common Name: Bromine Empirical Formula: Br2	CAS Number: 7726-95-6

Sorptive Properties

Filter Performance Index: Poor

Physical Adsorption: Weak to moderate adsorption on activated carbon. Water soluble, desorption may decrease or be delayed with increasing relative humidity and adsorbed water.

Chemisorption: Possible removal by NBC filters due to hydrolysis and reaction with metal impregnants.

Physical Properties

Molecular Weight:	159.82
Boiling Point:	58.8 C
Vapor Pressure:	73 mmHg at 0C, 175 mmHg at 21 C, 200 mmHg at 24.3 C, 400 mmHg at 41 C, 1520 mmHg at 78.8 C, 2279 mmHg at 110.3 C, Antoine: T=224.4-331.3 K A=2.94529 B=638.258 C=-115.133, T=343-383K A=4.70827 B=1562.264 C=0.628 (T=K, LogP=bar, NIST), A=15.8441 B=2582.32 C=-51.56 (T=K, LnP=mm Hg, Praisnitz)
Volatility:	5.5 (air=1)
Critical Temperature:	315 C
Critical Pressure:	102 atm
Heat of Vaporization:	43.7 cal/g
Solubility in Water:	35.8 g/L at 20C
Liquid Density:	3.1023 g/cm at 25C, 2.928 g/cm3 at 59C

Toxicity

ACGIH TLV-TWA: 0.1 ppm	NIOSH REL-TWA:	OSHA PEL: 0.65 mg/m3
ACGIH TLV-STEL: 0.3 ppm	NIOSH REL-STEL:	

References

1. IUCLID Data Sheet
2. NIST Chemistry WebBook
3. MSDS, Howard Hughes Medical institute
4. The Merck Index, 11th Edition
5. Prausnitz
6. hhmi.org web site
7. Handbook of Chemistry and Physics

Chemical Name	Hazard Index: Low
Common Name: bromine chloride Empirical Formula: BrCl	CAS Number: 13863-41-7

Sorptive Properties

Filter Performance Index: Marginal

Physical Adsorption: Weakly adsorbed on activated carbon due to high vapor pressure, unstable gas.

Chemisorption: Possible removal by NBC filters due to hydrolysis and reaction with metal impregnants

Physical Properties

Molecular Weight: 115.36
Boiling Point: decomposes at ca. 5 C
Vapor Pressure:

Volatility: 5.0 g/L
Critical Temperature:
Critical Pressure:
Heat of Vaporization:
Solubility in Water:
Liquid Density:

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

Chemical Name	Hazard Index: Low
Common Name: Bromine Pentafluoride Empirical Formula: BrF5	CAS Number: 7789-30-2

Sorptive Properties

Filter Performance Index: Marginal

Physical Adsorption: Weakly adsorbed on activated carbon. Water reactive.

Chemisorption: Possible removal by NBC filters due to hydrolysis and reaction with metal impregnants

Physical Properties

Molecular Weight:	174.9
Boiling Point:	40.76
Vapor Pressure:	ca. 397 mm Hg at 25 C, Antoine: T=203.8-313.5 K A=4.79777 B=1411.692 C=-19.763 (T=K, LogP=bar, NIST)
Volatility:	6.05 (air=1)
Critical Temperature:	197 C
Critical Pressure:	
Heat of Vaporization:	42.7 cal/g
Solubility in Water:	exploseds on contact with water
Liquid Density:	2.46 g/mL at 25 C

Toxicity

ACGIH TLV-TWA: 0.7 mg/m3	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook
2. The Merck Index, 11th Edition

Chemical Name	Hazard Index: Low
Common Name: Bromine trifluoride Empirical Formula:	CAS Number: 7787-71-5

Sorptive Properties

Filter Performance Index: Marginal

Physical Adsorption: Marginal to strong adsorption on activated carbon.

Chemisorption: Possible removal by NBC filters due to hydrolysis and reaction with metal impregnants

Physical Properties

Molecular Weight:	136.9
Boiling Point:	125.8
Vapor Pressure:	6.1 mm Hg at 22 C
Volatility:	4.7
Critical Temperature:	327 C
Critical Pressure:	
Heat of Vaporization:	74 cal/g
Solubility in Water:	
Liquid Density:	2.81 g/mL at 20 C

Toxicity

ACGIH TLV-TWA: 2.5 mg/m3	NIOSH REL-TWA: 2.5 mg/m3	OSHA PEL: 2.5 mg/m3
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

Chemical Name	Hazard Index: Low
Common Name: Carbonyl Fluoride Empirical Formula: CF2O	CAS Number: 353-50-4

Sorptive Properties

Filter Performance Index: Poor

Physical Adsorption: Weakly adsorbed on activated carbon due to high vapor pressure

Chemisorption: unknown (Kaufman, 1945 on carbonyls). Reacts in water

Physical Properties

Molecular Weight:	66.01
Boiling Point:	-83.1 C
Vapor Pressure:	Antoine: T=163.6-189.17 K, A=3.9959 B=572.866 C=-45.011(T=K, LogP=bar, NIST)
Volatility:	2.29 (air=1)
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	
Solubility in Water:	hydrolyzes
Liquid Density:	1.139 g/mL at 25C

Toxicity

ACGIH TLV-TWA: 5.4 mg/m3	NIOSH REL-TWA: 5.4 mg/m3	OSHA PEL: 5.4 mg/m3
ACGIH TLV-STEL: 13.4 mg/m3	NIOSH REL-STEL: 13.4 mg/m3	

References

1. NIST Chemistry WebBook
2. MSDS, Environmental Chemicals Data and Information Network
3. The Merck Index, 11th Edition
4. Handbook of Chemistry and Physics

Chemical Name	Hazard Index: Low
Common Name: chlorine pentafluoride Empirical Formula: ClF5	CAS Number: 13637-63-3

Sorptive Properties

Filter Performance Index: Marginal

Physical Adsorption: Weakly adsorbed on activated carbon due to high vapor pressure.

Chemisorption: Likely removal by NBC filters due to hydrolysis and reaction with metal impregnants. Reactions probably similar to chlorine trifluoride, fluorine, chlorine and boron trifluoride. (Bohart, 1920 on chlorine, Dickinson , 1942, Emmett, 1943 on BF3, Rogge, 1959 on chlorine)

Physical Properties

Molecular Weight: 130.44

Boiling Point: -13.1 C

Vapor Pressure: ca. 2876 mm Hg at 25 C, Antoine: T=193.9-297.9 K, A=3.76103 B=798.006 C=-46.838 (T=K, LogP=bar, NIST)

Volatility:

Critical Temperature:

Critical Pressure:

Heat of Vaporization:

Solubility in Water:

Liquid Density:

Toxicity

ACGIH TLV-TWA: 2.5 mg/m3	NIOSH REL-TWA: 2.5 mg/m3	OSHA PEL: 2.5 mg/m3
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook

Chemical Name	Hazard Index: Low
Common Name: Chlorine Trifluoride Empirical Formula: ClF3	CAS Number: 7790-91-2

Sorptive Properties

Filter Performance Index: Marginal

Physical Adsorption:	Weakly adsorbed on activated carbon due to high vapor pressure. Highly reactive in water.
Chemisorption:	Likely removal by NBC filters due to hydrolysis and reaction with metal impregnants. Reactions probably similar to ClF5.

Physical Properties

Molecular Weight:	92.45
Boiling Point:	11.75 C
Vapor Pressure:	1211mm Hg at 25 C, Antoine: T=192.7-284.6 K A=4.31282 B=1182.409 C=-10.335 (T=K, LogP=bar, NIST)
Volatility:	.235 (air=1)
Critical Temperature:	153 C
Critical Pressure:	56.9 atm
Heat of Vaporization:	71.2 cal/g
Solubility in Water:	violently hydrolyzed
Liquid Density:	1.77 at 13 C

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA: 0.37 mg/m3	OSHA PEL: 0.37 mg/m3
ACGIH TLV-STEL: 0.37 mg/m3	NIOSH REL-STEL:	

References

1. MSDS, Liquid Air Corporation, January 1, 1987
2. NIST Chemistry WebBook
3. The Merck Index, 11th Edition
4. Handbook of Chemistry and Physics

Chemical Name	Hazard Index: Low
Common Name: Chloroacetaldehyde Empirical Formula: C2H3ClO	CAS Number: 107-20-0

Sorptive Properties

Filter Performance Index: Marginal

Physical Adsorption: Strong to moderate adsorption on activated carbon, delayed desorption under dry conditions. Water soluble, desorption may decrease or be delayed with increasing relative humidity and adsorbed water.

Chemisorption: unknown

Physical Properties

Molecular Weight: 78.50

Boiling Point: 85 C

Vapor Pressure: 100 mm Hg at 45 C, ca. 35 mm Hg at 25 C

Volatility:

Critical Temperature:

Critical Pressure:

Heat of Vaporization:

Solubility in Water: 100 mg/mL at 19 C

Liquid Density: 1.236 g/mL in 50% aqueous solution

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA: 3.2 mg/m3	OSHA PEL: 3.2 mg/m3
ACGIH TLV-STEL: 3.2 mg/m3	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook
2. MSDS, Radian Corporation, August 29,1991

Chemical Name	Hazard Index: Low
Common Name: Chloroacetyl Chloride Empirical Formula: C2H2Cl2O	CAS Number: 79-04-9

Sorptive Properties

Filter Performance Index:	Marginal
Physical Adsorption:	Moderate to strong adsorption on activated carbon, delayed desorption likely under dry conditions. Effect of adsorbed water unknown.
Chemisorption:	unknown

Physical Properties

Molecular Weight:	112.94
Boiling Point:	106 C
Vapor Pressure:	19.64 mmHg at 20 C, Antoine: T=301.48-380.22 K A=4.2622 B=1333.71 C=-65.791 (T=K, LogP=bar, NIST)
Volatility:	
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	92 cal/g
Solubility in Water:	
Liquid Density:	1.418 g/ml at 20 C

Toxicity

ACGIH TLV-TWA: 0.2 mg/m3	NIOSH REL-TWA: 0.2 mg/m3	OSHA PEL: 0.2 mg/m3
ACGIH TLV-STEL: 0.7 mg/m3	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook
2. The Merck Index, 11th Edition
3. Aldrich

Chemical Name	Hazard Index: Low
Common Name: Cyanogen Empirical Formula: C2N2	CAS Number: 460-19-5

Sorptive Properties

Filter Performance Index: Effective

Physical Adsorption: Weakly adsorbed on activated carbon. Water soluble.

Chemisorption: Effective removal by NBC filters due to reaction with metal impregnants

Physical Properties

Molecular Weight:	52.03
Boiling Point:	-21.17 C
Vapor Pressure:	4240 mm Hg at 25 C, Antoine: T=252-391 K A=4.51661 B=1041.518 C=-21.288 (T=K, LogP=bar, NIST)
Volatility:	
Critical Temperature:	126.6 C
Critical Pressure:	58.2 atm
Heat of Vaporization:	5.778 kcal/mole
Solubility in Water:	1 volume of H2O dissolves 4 volumes of cyanogen gas
Liquid Density:	0.9537 g/mL at -boiling point

Toxicity

ACGIH TLV-TWA: 21 mg/m3	NIOSH REL-TWA: 21 mg/m3	OSHA PEL: 21 mg/m3
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook
2. The Merck Index, 11th Edition

Chemical Name	Hazard Index: Low
Common Name: diphenylmethane-4,4'-diisocyanat	
Empirical Formula: C15H10N2O2	CAS Number: 101-68-8

Sorptive Properties

Filter Performance Index:	Effective
Physical Adsorption:	Strong adsorption on activated carbon.
Chemisorption:	unknown

Physical Properties

Molecular Weight:	250.26
Boiling Point:	314 C
Vapor Pressure:	5.0E-6 mm Hg at 25 C,Antoine: T=442-530 K, A=2.41991 B=969.926 C=-253.28 (T=K, LogP=bar, NIST)
Volatility:	>1.0 (air=1)
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	
Solubility in Water:	
Liquid Density:	1.23 g/mL at 25 C

Toxicity

ACGIH TLV-TWA: 0.05 mg/m3	NIOSH REL-TWA: 0.05 mg/m3	OSHA PEL: 0.20 mg/m3
ACGIH TLV-STEL:	NIOSH REL-STEL: 0.2 mg/m3	

References

1. NIST Chemistry WebBook
2. www.pdc.cornell.edu/msds
3. 1997 Beilstein CD&S Reg No. 797662

Chemical Name	Hazard Index: Low
Common Name: Ethyl Chloroformate Empirical Formula: C3H5ClO2	CAS Number: 541-41-3

Sorptive Properties

Filter Performance Index: Marginal

Physical Adsorption: Moderate to strong adsorption on activated carbon, delayed desorption under dry conditions. Decomposes in water.

Chemisorption: unknown

Physical Properties

Molecular Weight: 108.52
Boiling Point: 93-95C
Vapor Pressure: 41 mmHg at 20 C

Volatility:
Critical Temperature:
Critical Pressure:
Heat of Vaporization:
Solubility in Water: decomposes
Liquid Density: 1.1403 g/mL at 20 C

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook
2. The Merck Index, 11th Edition
3. MSDS, Fisher Corp
4. Aldrich

Chemical Name	Hazard Index: Low
Common Name: ethyl chlorothioformate Empirical Formula: C3H5ClOS	CAS Number: 2941-64-2

Sorptive Properties

Filter Performance Index:	Effective
Physical Adsorption:	Strong adsorption on activated carbon, delayed desorption likely under dry. Effect of adsorbed water unknown.
Chemisorption:	unknown

Physical Properties

Molecular Weight:	124.58
Boiling Point:	136 C
Vapor Pressure:	
Volatility:	
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	
Solubility in Water:	
Liquid Density:	1.84 g/mL at 16C

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. Beilstein 773809 (1998)

Chemical Name		Hazard Index: Low
Common Name: Ethylene Amine Empirical Formula: C2H5N		CAS Number: 593-67-9

Sorptive Properties

Filter Performance Index: Poor

Physical Adsorption: Weak to moderate adsorption on activated carbon, desorption likely under dry conditions. Water soluble, desorption may decrease or be delayed with increasing realtive humidity and co-adsorbed water.

Chemisorption: unknown

Physical Properties

Molecular Weight: 43.07

Boiling Point: 329.8

Vapor Pressure: 160 mmHg at 20 C, Antoine: T=270-400 K, A=16.4227 B=2610.44 C=-63.15 (T=K, LnP=mm Hg, Prausnitz)

Volatility:

Critical Temperature:

Critical Pressure:

Heat of Vaporization:

Solubility in Water: highly soluble

Liquid Density: 0.833 g/mL at 293 K

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook
2. MSDS, New Jersey Dept of Health, October 1986
3. Prausnitz

Chemical Name	Hazard Index: Low
Common Name: ethylphosphonothioic dichloride Empirical Formula: C2H5Cl2PS	CAS Number: 993-43-1

Sorptive Properties

Filter Performance Index: Effective

Physical Adsorption: Strong adsorption on activated carbon.

Chemisorption: unknown

Physical Properties

Molecular Weight: 163
Boiling Point: 82.5 C at 45.5 torr
Vapor Pressure: ca. 1-4 mm Hg at 25 C

Volatility:
Critical Temperature:
Critical Pressure:
Heat of Vaporization:
Solubility in Water:
Liquid Density:

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. 1997 Beilstein CD&S Reg No. 1743462

Chemical Name	Hazard Index: Low
Common Name: ethylphosphonous dichloride Empirical Formula: C2H5Cl2P	CAS Number: 1498-40-4

Sorptive Properties

Filter Performance Index:	Marginal
Physical Adsorption:	Moderate to strong adsorption on activated carbon, delayed desorption under dry conditions. Effect of adsorbed water unknown
Chemisorption:	unknown

Physical Properties

Molecular Weight:	130.94
Boiling Point:	113 C at 752 mm Hg
Vapor Pressure:	ca. 35 mm Hg at 25 C
Volatility:	
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	
Solubility in Water:	
Liquid Density:	

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook
2. 1997 Beilstein CD&S Reg No. 906709

Chemical Name	Hazard Index: Low
Common Name: hexachlorocyclopentadiene	
Empirical Formula: C5Cl6	CAS Number: 77-47-4

Sorptive Properties

Filter Performance Index:	Effective
Physical Adsorption:	Strong adsorption on activated carbon.
Chemisorption:	unknown

Physical Properties

Molecular Weight:	272.76
Boiling Point:	239 C at 753 mmHg
Vapor Pressure:	0.1 mmHg at 298K
Volatility:	9.42 (air=1)
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	
Solubility in Water:	soluble, 0.13 mg/l at 25C
Liquid Density:	1.702 g/mL

Toxicity

ACGIH TLV-TWA: 0.1 mg/m3	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. www.fisher1.com/
2. haz1.siri.org/msds/

Chemical Name	Hazard Index: Low
Common Name: Hydrogen Iodide Empirical Formula: HI	CAS Number: 10034-85-2

Sorptive Properties

Filter Performance Index: Poor

Physical Adsorption:	Weakly adsorbed on activated carbon due to high vapor pressure. Water soluble.
Chemisorption:	Likely removal by NBC filters due to hydrolysis and reaction with metal impregnants. Chemisorption similar to HBr and HCl.

Physical Properties

Molecular Weight:	127.91
Boiling Point:	-35.1 C
Vapor Pressure:	4147 mmHg at 20C, 7600 mmHg at 32C, Antoine: T=149.8-238K A=4.26854 B=939.994 C=-18.012 (T=K, LogP=bar,NIST), T=215-256 K, A=12.9149 B=957.96 C=-85.06 (T=K, LnP=mm Hg, Prausnitz)
Volatility:	
Critical Temperature:	151 C
Critical Pressure:	82 atm
Heat of Vaporization:	
Solubility in Water:	234 g/100g H2O at 10C, 900 g/100g H2O at 0 C
Liquid Density:	2.803 g.mL at 237 K, 5.23 g/l at 25 C

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook
2. The Merck Index, 11th Edition
3. Handbook of Chemistry and Physics
4. Prausnitz

Chemical Name	Hazard Index: Low
Common Name: isobutyl chloroformate Empirical Formula: C5H9ClO2	CAS Number: 543-27-1

Sorptive Properties

Filter Performance Index: Marginal

Physical Adsorption: Moderate to strong adsorption on activated carbon, delayed desorption under dry conditions. Effect of adsorbed water unknown.

Chemisorption: unknown

Physical Properties

Molecular Weight: 136.58
Boiling Point: 129 C
Vapor Pressure: 25-30 mm Hg at 25 C

Volatility:
Critical Temperature:
Critical Pressure:
Heat of Vaporization:
Solubility in Water:
Liquid Density:

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook

Chemical Name	Hazard Index: Low
Common Name: isopropyl chloroformate Empirical Formula: C4H7ClO2	CAS Number: 109-61-5

Sorptive Properties

Filter Performance Index:	Marginal
	Moderate adsorption on activated carbon followed by desorption under dry conditions. Effect of adsorbed water unknown
Chemisorption:	Unknown

Physical Properties

Molecular Weight:	122.55
Boiling Point:	115.3 C
Vapor Pressure:	ca. 30-40 mm Hg at 25 C
Volatility:	4.2 (air=1)
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	
Solubility in Water:	
Liquid Density:	1.08 g/mL

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook

Chemical Name	Hazard Index: Low
Common Name: isopropyl isocyanate Empirical Formula: C4H7NO	CAS Number: 1795-48-8

Sorptive Properties

Filter Performance Index: Poor

Physical Adsorption: Weak to moderate adsorption on activated carbon, desorption likely under dry conditions. Effect of adsorbed water unknown.

Chemisorption: unknown

Physical Properties

Molecular Weight: 85.11
Boiling Point: 68-69 C
Vapor Pressure: 100 mmHg at 25 C

Volatility:
Critical Temperature:
Critical Pressure:
Heat of Vaporization:
Solubility in Water:
Liquid Density: 0.8669 g/cm3 at 20 C

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. 1998 Beilstein CD&S, 969356

Chemical Name	Hazard Index: Low
Common Name: n-propyl chloroformate Empirical Formula: C4H7ClO2	CAS Number: 109-61-5

Sorptive Properties

Filter Performance Index: Marginal

Physical Adsorption: Moderate to strong adsorption on activated carbon, delayed desorption under dry conditions. Effect of adsorbed water unknown.

Chemisorption: unknown

Physical Properties

Molecular Weight: 122.55
Boiling Point: 115.3 C
Vapor Pressure: 20 mmHg at 20C

Volatility:
Critical Temperature:
Critical Pressure:
Heat of Vaporization:
Solubility in Water:
Liquid Density:

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook
2. Aldrich
3. CRC Press, 1989

Chemical Name	Hazard Index: Low
Common Name: n-propyl chloroformate	
Empirical Formula: C4H7ClO2	CAS Number: 109-61-5

Sorptive Properties

Filter Performance Index:	Marginal
Physical Adsorption:	Strong to moderate adsorption on activated carbon, delayed desorption under dry conditions. Effect of adsorbed water unknown.
Chemisorption:	unknown

Physical Properties

Molecular Weight:	122.5
Boiling Point:	115.2 C
Vapor Pressure:	ca 35 mm Hg at 25 C
Volatility:	
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	
Solubility in Water:	
Liquid Density:	1.0901 at 20 C

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. haz1.siri.org:80/msds/

Chemical Name	Hazard Index: Low
Common Name: Nitric Oxide Empirical Formula: NO	CAS Number: 10102-43-9

Sorptive Properties

Filter Performance Index: Poor

Physical Adsorption: Weakly adsorbed on activated carbon undry and humid conditions

Chemisorption: Reacts readily with air to produce nitrogen dioxide, which is chemisorbed to a limited extent. NO may be converted to NO2 by NBC filters.

Physical Properties

Molecular Weight:	30.01
Boiling Point:	-151.8 C
Vapor Pressure:	Antoine: T= 95-140 K, A=20.1314 B=1572.52 C=-4.88 (T=K, LnP=mm Hg, Prausnitz)
Volatility:	1.04 (air=1)
Critical Temperature:	-94 C
Critical Pressure:	49400 mmHg
Heat of Vaporization:	3.293kcal/mole at boiling point
Solubility in Water:	4.6 mL/100mL at 20 C, 2.37mL/100mL at 60 C
Liquid Density:	1.27 at -150.2 C

Toxicity

ACGIH TLV-TWA: 30 mg/m3	NIOSH REL-TWA: 30 mg/m3	OSHA PEL: 30 mg/m3
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. MSDS, Liquid Air Corporation, January 1, 1987
2. The Merck Index, 11th Edition
3. NIST Chemistry WebBook
4. Prausnitz

Chemical Name	Hazard Index: Low
Common Name: parathion Empirical Formula: C10H14NO5PS	CAS Number: 56-38-2

Sorptive Properties

Filter Performance Index:	Effective
Physical Adsorption:	Strong adsorption on activated carbon. Desorption may increase with increasing relative humidity and adsorbed water.
Chemisorption:	unknown

Physical Properties

Molecular Weight:	291
Boiling Point:	375 C
Vapor Pressure:	3.78x10-5 mmHg at 20 C
Volatility:	1.262 (air=1)
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	
Solubility in Water:	insoluble
Liquid Density:	

Toxicity

ACGIH TLV-TWA: 0.1 mg/m3	NIOSH REL-TWA: 0.05 mg/m3	OSHA PEL: 0.1 mg/m3
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook
2. www.pdc.cornell.edu/msds/hazcom/

Chemical Name	Hazard Index: Low
Common Name: perchloromethyl mercaptan Empirical Formula: CCl4S	CAS Number: 594-42-3

Sorptive Properties

Filter Performance Index: Effective

Physical Adsorption: Strong adsorption on activated carbon. Effect of adsorbed water unknown

Chemisorption: unknown

Physical Properties

Molecular Weight: 185.88
Boiling Point: 149C
Vapor Pressure: 10 mm Hg at 30 C

Volatility:
Critical Temperature:
Critical Pressure:
Heat of Vaporization:
Solubility in Water:
Liquid Density: 1.7 g/mL at 12.8 C

Toxicity

ACGIH TLV-TWA: 0.8 mg/m3	NIOSH REL-TWA: 0.8 mg/m3	OSHA PEL: 0.8 mg/m3
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. Smith; Delin, Svan.Kem.Tidskr., 65<1953>10, 15, CODEN:SKTIAF
2. Rathke, Justus Liebigs Ann. Chem., 167 <1873>, 199, CODEN:JLACBF

Chemical Name	Hazard Index: Low
Common Name: sec-butyl chloroformate Empirical Formula: C5H9ClO2	CAS Number: 17462-58-7

Sorptive Properties

Filter Performance Index:	Marginal
Physical Adsorption:	Moderate adsorption on activated carbon, delayed desorption under dry conditions. Effect of adsorbed water unknown.
Chemisorption:	unknown

Physical Properties

Molecular Weight:	136.58
Boiling Point:	121-124 C at 748 mm Hg
Vapor Pressure:	ca. 12-30 mm Hg at 25 C
Volatility:	
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	
Solubility in Water:	
Liquid Density:	

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. 1997 Beilstein CD&S Reg No. 506645

Chemical Name	Hazard Index: Low
Common Name: Sulfuryl Fluoride Empirical Formula: F2O2S	CAS Number: 2699-79-8

Sorptive Properties

Filter Performance Index: Poor

Physical Adsorption: Weakly adsorbed on activated carbon due to high vapor pressure. Desorption may increase with increasing relative humidity and adsorbed water.

Chemisorption: unknown

Physical Properties

Molecular Weight:	102.06
Boiling Point:	-55 C
Vapor Pressure:	9150 mmHg at 10 C
Volatility:	3.72 g/l
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	45.03 cal/g
Solubility in Water:	0.75g/kg at 25C
Liquid Density:	1.36 g/mL

Toxicity

ACGIH TLV-TWA: 20 mg/m3	NIOSH REL-TWA:	OSHA PEL: 20 mg/m3
ACGIH TLV-STEL: 40 mg/m3	NIOSH REL-STEL:	

References

1. US Dept of Labor, OSHA, January 15, 1993
2. University of Akron, Ohio
3. NIST Chemistry WebBook
4. MSDS, Extension Toxicology Network
5. The Merck Index, 11th Edition
6. Handbook of Chemistry and Physics

Chemical Name	Hazard Index: Low
Common Name: tert-butyl isocyanate Empirical Formula: C5H9NO	CAS Number: 1609-86-5

Sorptive Properties

Filter Performance Index:	Marginal
Physical Adsorption:	Moderate to strong adsorption on activated carbon, delayed desorption under dry conditions. Effect of adsorbed water unknown.
Chemisorption:	unknown (may be similar to methyl and iso-propyl isocyanates)

Physical Properties

Molecular Weight:	99.13
Boiling Point:	85C
Vapor Pressure:	13 mmHg at 298 K
Volatility:	
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	
Solubility in Water:	
Liquid Density:	0.83590 g/mL at 25C

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA:	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. 1998 Beilstein CD&S 969479

Chemical Name	Hazard Index: Low
Common Name: tetraethyl pyrophosphate Empirical Formula: C8H20O7P2	CAS Number: 107-49-3

Sorptive Properties

Filter Performance Index: Effective

Physical Adsorption: Strong adsorption on activated carbon, delayed desorption under dry conditions. Effect of adsorbed water unknown.

Chemisorption: unknown

Physical Properties

Molecular Weight: 290.19
Boiling Point: 155 C at 5 mm Hg
Vapor Pressure: 0.00038 mmHg at 298 K

Volatility:
Critical Temperature:
Critical Pressure:
Heat of Vaporization:
Solubility in Water:
Liquid Density: 1.18 g/mL at 25 C

Toxicity

ACGIH TLV-TWA: 0.05 mg/m3	NIOSH REL-TWA:	OSHA PEL: 0.05 mg/m3
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. 1997 Beilstein CD&S Reg No. 1714017

Chemical Name	Hazard Index: Low
Common Name: tetraethyllead Empirical Formula: C8H20Pb	CAS Number: 78-00-2

Sorptive Properties

Filter Performance Index: Effective

Physical Adsorption: Strong adsorption on activated carbon.

Chemisorption: unknown

Physical Properties

Molecular Weight:	323.44
Boiling Point:	~200 C
Vapor Pressure:	ca. 0.5 mm Hg at 25 C, Antoine: T=311.5-456 K, A=5.02305 B=1984.384 C=-60.506 (T=K, LogP= bar, NIST)
Volatility:	8.6 (air=1)
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	
Solubility in Water:	
Liquid Density:	1.653 g/mL

Toxicity

ACGIH TLV-TWA: 0.1 mg/m3	NIOSH REL-TWA:	OSHA PEL: 0.075 mg/m3
ACGIH TLV-STEL: 0.3 mg/m3	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook

Chemical Name	Hazard Index: Low
Common Name: tetramethyllead	
Empirical Formula: C4H12Pb	CAS Number: 75-74-1

Sorptive Properties

Filter Performance Index:	Marginal
Physical Adsorption:	Strong to moderate adsorption on activated carbon, delayed desorption under dry conditions. Effect of adsorbed water unknown.
Chemisorption:	unknown

Physical Properties

Molecular Weight:	267.34
Boiling Point:	101C
Vapor Pressure:	ca. 29 mm Hg at 25 C, Antoine: T=273-333 K A=4.14259 B=1376.726 C=-50.129 (T=K, LogP=bar, NIST)
Volatility:	6.5 (air=1)
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	30.8 cal/g
Solubility in Water:	
Liquid Density:	1.995 g/mL

Toxicity

ACGIH TLV-TWA: 0.15 mg/m3	NIOSH REL-TWA:	OSHA PEL: 0.075 mg/m3
ACGIH TLV-STEL: 0.5 mg/m3	NIOSH REL-STEL:	

References

1. NIST Chemistry WebBook
2. 1997 Beilstein CD&S Reg No. 3902986

Chemical Name	Hazard Index: Low
Common Name: toluene-2,4-diisocyanate Empirical Formula: C9H6N2O2	CAS Number: 584-84-9

Sorptive Properties

Filter Performance Index: Effective

Physical Adsorption: Strong adsorption on activated carbon.

Chemisorption: unknown

Physical Properties

Molecular Weight:	174.16
Boiling Point:	251 C
Vapor Pressure:	Antoine: T=293-443.2 K, A=4.59647 B=2064.243 C=-75.176 (T-K, LogP=bar, NIST), 0.016 mmHg at 298 K
Volatility:	6.0 (air=1)
Critical Temperature:	
Critical Pressure:	
Heat of Vaporization:	
Solubility in Water:	
Liquid Density:	1.224 g/mL

Toxicity

ACGIH TLV-TWA: 0.04 mg/m3	NIOSH REL-TWA: 0.035 mg/m3	OSHA PEL: 0.14 mg/m3
ACGIH TLV-STEL: 0.14 mg/m3	NIOSH REL-STEL:	

References

Chemical Name	Hazard Index: Low
Common Name: toluene-2,6-diisocyanate Empirical Formula: C9H6N2O2	CAS Number: 91-08-7

Sorptive Properties

Filter Performance Index: Effective

Physical Adsorption: Strong adsorption on activated carbon.

Chemisorption: unknown

Physical Properties

Molecular Weight: 174.16
Boiling Point: 101-103C at 6 mm Hg,
Vapor Pressure: 0.5 mm Hg at 25 C

Volatility:
Critical Temperature:
Critical Pressure:
Heat of Vaporization:
Solubility in Water:
Liquid Density: 1.22 g/mL at 25 C

Toxicity

ACGIH TLV-TWA:	NIOSH REL-TWA: 0.035 mg/m3	OSHA PEL:
ACGIH TLV-STEL:	NIOSH REL-STEL:	

References

1. Beilstein 2211546 (1998)